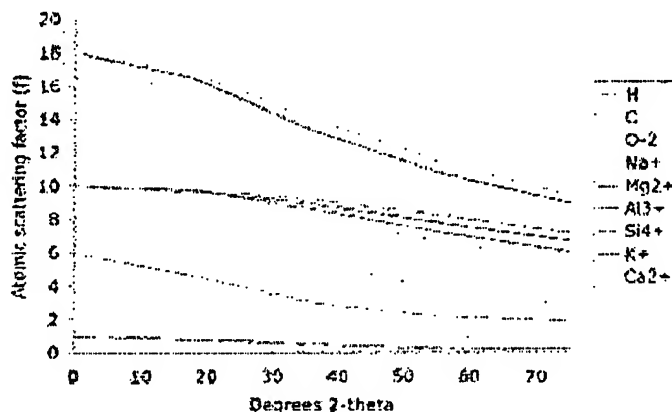


## APPENDIX B

As a consequence,  $f'$  decreases with increasing angle of reflection. The figure below shows the change in  $f'$  for commonly encountered ions in clay minerals. The values are plotted as a function to degrees two-theta. The plot below is for Cu K $\alpha$  radiation. Click [here](#) for an Excel spreadsheet that allows you to change the wavelength of radiation (data from Cullity, 1978).



### Scattering from a unit cell

Recall that rows of atoms cause scatter in specific directions resulting in constructive interference or coherent scatter.

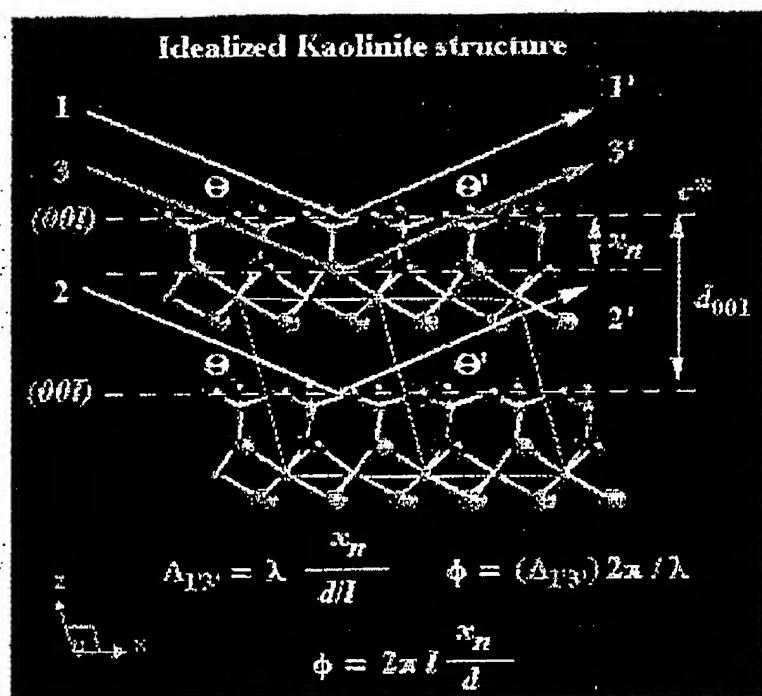
For the case of clay minerals, the approach is greatly simplified. The morphological nature of clay minerals is such that they can easily be prepared to orient their crystallographic axes (the  $ab$  plane) relative to the X-ray beam. This is called "preferred orientation" (as opposed to random orientation).

We now want to describe this diffraction effect from a unit cell in a crystal. If the clays are oriented, then we can consider this to be a one-dimensional diffraction problem.

The scattering from a unit cell ( $F$ ) is always less than the total sum of atoms in the unit cell because the rays that the atoms scatter are out of phase with each other.  $F$  is called the structure factor and is therefore, a measure of the intensity of the diffracted X-ray beam.

To find  $F$ , the sum of the amplitudes of each atom in the unit cell must be determined.

The sum of amplitudes must be adjusted by the amount of phase difference due to the location of the atoms in the unit cell. Recall that the phase difference is related to (1) the wavelength, (2) the angle of incidence, (3) the position of the atom planes and (4) the number and type of atoms in each plane. An example is given in the figure below.



Phase shift  $\phi$  can be expressed in more common crystallographic variables.

If  $d$  is the  $c$  lattice parameter, and  $x/c$  is the fractional coordinate  $w$  (recall also that  $(uvw)$  are the fractional coordinates for any position within a 3-D unit cell), then the phase shift expression becomes

$$\phi = 2\pi l w$$

For the 3-D case (i.e.,  $(hkl)$ )

$$\phi = 2\pi (h u + k v + l w)$$

Phase differences between the scattered waves (all with the same wavelength) can be determined mathematically by a structure factor function where:

$$F = \sum_n f_n \exp(i \phi_n) = f \exp(i \phi_1) + f \exp(i \phi_2) + \dots f \exp(i \phi_n)$$

where:

- $F$  – amplitude or structure factor
- $f$  – atomic scattering factor
- $\phi$  – phase angle
- $i = \text{sqrt}(-1)$
- $n$  – atom type

We use the identity: